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1RQI

DOI 10.2210/pdb1rqI/pdb

Images :

Red - Derived Information

Title

Active Conformation of Farnesyl Pyrophosphate Synthase Bound to Isopentenyl Pyrophosphate and Dimethylallyl S-Thiolodiphosphate

Authors
Hosfield, D.J., Zhang, Y., Dougan, D.R., Brooun, A., Tari, L.W., Swanson, R.V., Finn, J.

Primary Citation
Hosfield, D.J., Zhang, Y., Dougan, D.R., Brooun, A., Tari, L.W., Swanson, R.V., Finn, J. Structural basis for bisphosphonate-mediated inhibition of isoprenoid biosynthesis *J.Biol.Chem.* v279 pp.8526-8529, 2004

[Abstract]

History
Deposition 2003-12-05 Release 2004-03-02

Experimental Method
Type X-RAY DIFFRACTION Data N/A

Parameters
Resolution[Å] R-Value R-Free Space Group
2.42 0.206 (obs.) 0.259 P 4₁ 2 2

Unit Cell
Length [Å] a 88.84 b 88.84 c 174.77
Angles [°] alpha 90.00 beta 90.00 gamma 90.00

Molecular Description
Asymmetric Unit












Polymer: 1 Molecule: Geranyltranstransferase Chains: A,B EC no.: 2.5.1.10

Classification **Transferase**

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Source	Polymer: 1	Scientific Name: Escherichia coli	 Common Name: Bacteria	Expression system: Esc		
Chemical Component	Identifier	Name	Formula	Drug Similarity	Hapten Similar	
MG	IPR	MAGNESIUM ION	Mg ²⁺			
	DST	ISOPENTYL PYROPHOSPHATE	C ₅ H ₁₄ O ₇ P ₂			
	DPO	DIMETHYLLALLYL S-THIOLODIPHOSPHATE	C ₅ H ₁₄ O ₆ P ₂ S			
		DIPHOSPHATE	O ₇ P ₂ ⁴⁻			
SCOP Classification (version 1.71)	Domain Info	Class	Fold	Superfamily	Family	Domain
d1rqia_	All alpha proteins	Terpenoid synthases	Terpenoid synthases	Terpenoid synthases	Isoprenyl diphosphate synthases	Farnesyl diph synthase (geranyltrans
	d1rqib_	All alpha proteins	Terpenoid synthases	Terpenoid synthases	Isoprenyl diphosphate synthases	Farnesyl diph synthase (geranyltrans
CATH Classification (version v3.0.0)	Domain	Class	Architecture	Topology		
1rqIA00	Mainly Alpha	Orthogonal Bundle	Farnesyl Diphosphate Synthase			
1rqIB00	Mainly Alpha	Orthogonal Bundle	Farnesyl Diphosphate Synthase			
PFAM Classification	Chain	PFAM Accession	PFAM ID	Description	Type	
A	PF00348 	polyprenyl_synt	Polyprenyl synthetase	Domain		
B	PF00348 	polyprenyl_synt	Polyprenyl synthetase	Domain		
GO Terms	Polymer	Molecular Function	Biological Process			
Geranyltransferase (1RQI:A,B)	• none	• isoprenoid biosynthetic process				

WEST Search History

DATE: Friday, March 23, 2007

Hide?	<u>Set Name</u>	<u>Query</u>	<u>Hit Count</u>
		<i>DB=PGPB,USPT,USOC,EPAB,JPAB,DWPI; PLUR=YES; OP=ADJ</i>	
<input type="checkbox"/>	L7	L1 and (Brooun\$ or Dougan\$ or Hosfield\$ or Zhang\$).in.	10
<input type="checkbox"/>	L6	L1 and ispA	9
<input type="checkbox"/>	L5	L4 and ispA	2
<input type="checkbox"/>	L4	L3 and coordinate	61
<input type="checkbox"/>	L3	L2 and coli	164
<input type="checkbox"/>	L2	L1 and crystal structure	198
<input type="checkbox"/>	L1	farnesyl and synthase and crystal	501

END OF SEARCH HISTORY

STN

10651668

=> d his

(FILE 'HOME' ENTERED AT 14:50:27 ON 23 MAR 2007)

FILE 'CAPLUS' ENTERED AT 14:50:44 ON 23 MAR 2007

L1 57 S FARNESYL AND SYNTHASE AND CRYSTAL

L2 2 S L1 AND ISPA

=> d L2 1-2

L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:1178062 CAPLUS

DN 143:418026

TI Pseudomonas aeruginosa gene ispA farnesyl diphosphate
synthase, its cloning, and biochem. and biophys. characterization
useful for drug design

IN Edwards, Aled; Dharamsi, Akil; Vedadi, Masoud; Kimber, Matthew; Vallee,
Francois

PA Affinium Pharmaceuticals, Inc., Can.

SO U.S. Pat. Appl. Publ., 154 pp., Cont.-in-part of Appl. PCT/CA03/00714.
CODEN: USXXCO

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	US 2005245728	A1	20051103	US 2004-967671	20041018
	WO 2003097789	A2	20031127	WO 2003-CA714	20030521
	WO 2003097789	A3	20040205		
PRAI	US 2002-382443P	P	20020521		
	WO 2003-CA714	A2	20030521		

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2003:931464 CAPLUS

DN 140:2343

TI Cloning and physical characterization of farnesyl diphosphate
synthase from Pseudomonas aeruginosa and its use as a
antimicrobial target

IN Edwards, Aled; Dharamsi, Akil; Vedadi, Masoud; Mansoury, Kamran; Houston,
Simon; Vallee, Francois; Kimber, Matthew

PA Affinium Pharmaceuticals, Inc., Can.

SO PCT Int. Appl., 240 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	WO 2003097789	A2	20031127	WO 2003-CA714	20030521
	WO 2003097789	A3	20040205		
	AU 2003229452	A1	20031202	AU 2003-229452	20030521
	US 2005245728	A1	20051103	US 2004-967671	20041018
PRAI	US 2002-382443P	P	20020521		
	WO 2003-CA714	W	20030521		

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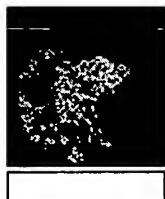
Help **34 Structure Hits** 8 Citations 28 Ligand Hits 2 Web Page Hits

1 2 3 4

☒ **1WCO**



THE SOLUTION STRUCTURE OF THE NISIN-LIPID II COMPLEX



Characteristics

Release Date: 07-Mar-2005 Exp. Method: NMR 20 Structu

Classification

Antibiotics

Compound

Polymer: 1 Molecule: ALA-DGL-LYS-DAL-DAL PEPT
Chains: L
Polymer: 2 Molecule: NISIN Chains: N Other
Details: THIOETHER BONDS (LANTHIONINE
LINKAGES) BETWEEN N3-N7, N8-N11, N13-N19, I
N26, N25-N28

Authors

Hsu, S.-T.D., Breukink, E., Tischenko, E., Lutter,
M.A.G., De Kruijff, B., Kaptein, R., Bonvin,
A.M.J.J., Van Nuland, N.A.J.

☒ **1ZW5**



X-ray structure of Farnesyl diphosphate synthase protein

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